=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
0.63 0.63

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 06:42:20 ON 25 JUL 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JUL 2006 HIGHEST RN 894992-91-7 DICTIONARY FILE UPDATES: 21 JUL 2006 HIGHEST RN 894992-91-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

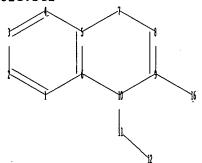
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10849559\10849559 best product core.str



chain nodes: 11 16

11 10

ring nodes :

1 2 3 4 5 6 7 8 9 10

ring/chain nodes :

12

chain bonds :

9-16 10-11 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

5-6 5-7 6-10 7-8 8-9 9-10 10-11 11-12

exact bonds :

9-16

normalized bonds :

Hydrogen count : 7:>= minimum 2 Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 16:CLASS

L1STRUCTURE UPLOADED

=> d 11L1 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam\ COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> search l1 sss sam SAMPLE SEARCH INITIATED 06:43:43 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 19412 TO ITERATE

10.3% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* \*\*COMPLETE\*\* BATCH

PROJECTED ITERATIONS: 379899 TO 396581

0 TO PROJECTED ANSWERS:

L2 0 SEA SSS SAM L1

=> search l1 sss full FULL SEARCH INITIATED 06:44:30 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 390464 TO ITERATE 100.0% PROCESSED 390464 ITERATIONS

SEARCH TIME: 00.00.02

L3 82 SEA SSS FUL L1

=> dscan

0 DSCAN

L4

0 DSCAN

=> d scan 13

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Ketone, 1-methoxy-1,3-diphenylinden-2-yl phenyl (7CI)

82 ANSWERS

MF C29 H22 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-1-ol, 2-ethyl-3-phenyl-, acetate (9CI)

MF C19 H18 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2,3-diethyl-1-methoxy- (9CI)

MF C14 H18 O

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2,3-diethyl-1,5-dimethoxy- (9CI)

MF C15 H20 O2

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzyl alcohol, o-[(1,4-dihydro-1-hydroxy-5,8-dimethoxy-2-naphthyl)methyl]-

, diacetate (6CI)

MF C24 H26 O6

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 7-[(1,1-dimethylethoxy)methyl]-2,3-diethyl-1-methoxy- (9CI)

MF C19 H28 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Indene, 1,7-dimethoxy-2,3-bis(1-methylethyl)- (9CI) MF C17 H24 O2

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Indene, 2,3-diethyl-1,5,7-trimethoxy- (9CI) MF C16 H22 O3

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

TN 1H-Indene-2-carboxamide. N-(aminoiminomethyl)-1-metho

IN 1H-Indene-2-carboxamide, N-(aminoiminomethyl)-1-methoxy-3-methyl-,
monomethanesulfonate (9CI)

MF C13 H15 N3 O2 . C H4 O3 S

CM 1

CM 2

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 9H-Fluorene, 9-[2-[(1,5,6,7-tetrahydro-2-methyl-s-indacen-1-yl)oxy]ethyl]-

(9CI)

MF C28 H26 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-(2-bromo-1-ethoxyethoxy)-4,7-dimethoxy-2,5-dimethyl-6-[2-

(phenylmethoxy)ethyl]-, (1S)- (9CI)

MF C26 H33 Br O5

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-1-ol, 6-methoxy-2-methyl-, acetate (9CI)

MF C13 H14 O3

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Propanoic acid, 2,2-dimethyl-, 6-methoxy-2-methyl-1H-inden-1-yl ester

(9CI)

MF C16 H20 O3

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN lH-Indene, 1-[(1S)-2-bromo-1-ethoxyethoxy]-4,7-dimethoxy-2,5-dimethyl-6-[2-(phenylmethoxy)ethyl]-, (1S)-(9CI)

MF C26 H33 Br O5

Absolute stereochemistry. Rotation (+).

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Indene, 1-methoxy-2-methyl-1, 3-diphenyl- (4CI)

MF C23 H20 O

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Indeneacetic acid, 1-hydroxy-3-phenyl-, formate (4CI)

MF C18 H14 O4

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1,1-dimethoxy-2-methyl- (9CI)

MF C12 H14 O2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1,1-dibutoxy-2-propyl- (9CI)

MF C20 H30 O2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

#### L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene-2-carboxylic acid, 1,6-dimethoxy-3-phenyl-, ethyl ester (9CI)
MF C20 H20 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-1-ol, 2-hexyl-, acetate (9CI)

MF C17 H22 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 82 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-ethoxy-2-(2-ethoxyethyl)-3-phenyl- (9CI)

MF C21 H24 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> save temp 13 rawhetros/a
ANSWER SET L3 HAS BEEN SAVED AS 'RAWHETROS/A'

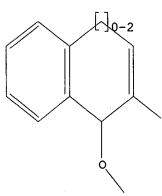
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10849559\10849559 core fixed H.str

chain nodes : 11 16 ring nodes : 1 2 3 4 5 6 7 8 9 10 ring/chain nodes : 12 chain bonds : 9-16 10-11 11-12 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 exact/norm bonds : 5-6 5-7 6-10 7-8 8-9 9-10 10-11 11-12 exact bonds : 9-16 normalized bonds : 1-2 1-6 2-3 3-4 4-5

Hydrogen count :
7:>= minimum 2 10:>= minimum 1
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 16:CLASS

#### L5 STRUCTURE UPLOADED

=> d 15 L5 HAS NO ANSWERS L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 15 subset=13 sss full FULL SUBSET SEARCH INITIATED 06:48:02 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED -82 TO ITERATE

100.0% PROCESSED 82 ITERATIONS 68 ANSWERS

SEARCH TIME: 00.00.01

L6 68 SEA SUB=L3 SSS FUL L5

=> d scan

REGISTRY COPYRIGHT 2006 ACS on STN L6 68 ANSWERS

Propanoic acid, 2,2-dimethyl-, 2-methyl-1H-inden-1-yl ester (9CI) IN

C15 H18 O2 MF

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

REGISTRY COPYRIGHT 2006 ACS on STN L6 68 ANSWERS

1H-Indene-3-d, 1-methoxy-2-methyl- (9CI) IN

MF C11 H11 D O

68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN L6

1H-Indene, 1,7-dimethoxy-2-methyl-3-phenyl- (9CI) IN

MF C18 H18 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-methoxy-2,5-dimethyl- (9CI)

MF C12 H14 O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-5-ol, 2,3-diethyl-1,7-dimethoxy-, acetate (9CI)

MF C17 H22 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-ethoxy-2-(2-ethoxyethyl)-6-fluoro-3-(4-fluorophenyl)- (9CI)

MF C21 H22 F2 O2

$$\begin{array}{c} \text{OEt} \\ \text{CH}_2\text{-}\text{CH}_2\text{-}\text{OEt} \\ \\ \text{F} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2,3-diethyl-1-methoxy-7-(2-methoxyethyl)- (9CI)

MF C17 H24 O2

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-1-ol, 2-pentyl-, acetate (9CI)

MF C16 H20 O2

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5H-Indeno[5,6-d]-1,3-dioxole, 6-butyl-5-methoxy- (9CI)

MF C15 H18 O3

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Palladium, dichloromethoxy(1-methoxy-2-methyl-1H-inden-3-yl)- (9CI)

MF C12 H14 C12 O2 Pd

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-1-ol, 2,3-dimethyl-, acetate (9CI)

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C16 H20 O3

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1-Acenaphthylenecarboxamide, 2-(acetyloxy)-2,6,7,8-tetrahydro- (9CI)

MF C15 H15 N O3

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Carbamic acid, bis(1-methylethyl)-, 2-methyl-1H-inden-1-yl ester (9CI)

MF C17 H23 N O2

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-methoxy-2,7-dimethyl- (9CI)

MF C12 H14 O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene-2-carboxamide, N-(aminoiminomethyl)-1-methoxy-3-methyl- (9CI)

MF C13 H15 N3 O2

CI COM

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2-methyl-1-(1-methylethoxy)- (9CI)

MF C13 H16 O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2,3-diethyl-1-methoxy-7-methyl- (9CI)

MF C15 H20 O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-1-ol, 2-hexyl-, acetate (9CI)

MF C17 H22 O2

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-methoxy-2-methyl- (9CI)

MF C11 H12 O

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1-Indenol, 2-methyl-3-(2-thienyl)-, acetate (5CI)

MF C16 H14 O2 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Indene, 2,3-diethyl-1,7-dimethoxy- (9CI)

MF C15 H20 O2

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C16 H20 O3

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Indene-2-carboxylic acid, 1-methoxy-3-methyl-, methyl ester (8CI)

MF C13 H14 O3

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-(2-bromo-1-ethoxyethoxy)-4,7-dimethoxy-2,5-dimethyl-6-[2-(phenylmethoxy)ethyl]-, (1S)- (9CI)

MF C26 H33 Br O5

### Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-methoxy-2,4-dimethyl- (9CI)

MF C12 H14 O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene-2-carboxamide, N-(aminoiminomethyl)-1-methoxy-3-methyl-,

monomethanesulfonate (9CI) MF C13 H15 N3 O2 . C H4 O3 S

CM 1

$$\begin{array}{c|c} \text{Me} & \text{O} & \text{NH} \\ \parallel & \parallel \\ \text{C-NH-C-NH}_2 \\ \\ \text{OMe} \end{array}$$

CM 2

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Indene, 2-methyl-1-(2-phenylethoxy)- (9CI)

MF C18 H18 O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1,7-dimethoxy-2,3-bis(1-methylethyl)- (9CI)

MF C17 H24 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-1-ol, 2,6-dimethyl-, acetate (9CI)

MF C13 H14 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzyl alcohol, o-[(1,4-dihydro-1-hydroxy-5,8-dimethoxy-2-naphthyl)methyl]-, diacetate (6CI)

MF C24 H26 O6

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Indeneacetic acid, 1-hydroxy-3-phenyl-, formate, 2,4-dinitrophenylhydrazone (4CI)

MF C24 H18 N4 O7

$$\begin{array}{c|c} Ph \\ \hline \\ CH_2-CO_2H \\ \hline \\ O-CH=N-NH \\ \hline \\ NO_2 \\ \end{array}$$

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2,3-diethyl-1-methoxy- (9CI)

MF C14 H18 O

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1,5-dimethoxy-2-methyl- (9CI)

MF C12 H14 O2

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene-2-carboxylic acid, 1-(acetyloxy)-, ethyl ester (9CI)

MF C14 H14 O4

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-1-ol, 2-methyl-, acetate (9CI)

MF C12 H12 O2

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 5-chloro-1-methoxy-2-methyl- (9CI)

MF C11 H11 Cl O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 3H-Benz[e]indene, 3-[2-(9H-fluoren-9-yl)ethoxy]-2-methyl- (9CI)

MF C29 H24 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-(2-bromoethoxy)-2-methyl- (9CI)

MF C12 H13 Br O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1,7-dimethoxy-2,3-dipentyl- (9CI)

MF C21 H32 O2

$$(CH_2)_4-Me$$
 $(CH_2)_4-Me$ 
OMe
OMe

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2-butyl-1-ethoxy- (9CI)
MF C15 H20 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Morpholine, 4-[[1-(acetyloxy)-3-(3,4-dimethoxyphenyl)-1H-inden-2yl]carbonyl]- (9CI)

MF C24 H25 N O6

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Indeneacetic acid, 1-hydroxy-3-phenyl-, formate (4CI)

MF C18 H14 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1,7-dimethoxy-2,3-dimethyl- (9CI)

MF C13 H16 O2

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1H-Indene, 1-(2-bromo-1-ethoxyethoxy)-2-methyl- (9CI)
MF C14 H17 Br O2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1H-Inden-1-ol, 5,7-dimethoxy-2,3-dimethyl-, acetate (9CI)
MF C15 H18 O4

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Inden-1-ol, 5-methoxy-2-methyl-, acetate (9CI) MF C13 H14 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Indene, 7-chloro-1-methoxy-2-methyl- (9CI)

MF C11 H11 Cl O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 9H-Fluorene, 9-[2-[(6,7,8,9-tetrahydro-2-methyl-3H-benz[e]inden-3-yl)oxy]ethyl]- (9CI)

MF C29 H28 O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2-ethyl-1-methoxy- (9CI)

MF C12 H14 O

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2,3-diethyl-1,4,7-trimethoxy- (9CI)

MF C16 H22 O3

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Indene, 1-ethoxy-2-(2-ethoxyethyl)-3-phenyl- (9CI) MF C21 H24 O2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1H-Indene, 2,3-diethyl-1-methoxy-7-(methoxymethyl)- (9CI)
MF C16 H22 O2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1H-Indene-2-carboxylic acid, 1,6-dimethoxy-3-phenyl-, ethyl ester (9CI)/
MF C20 H20 O4

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 7-(1,1-dimethylethoxy)-2,3-diethyl-1-methoxy- (9CI)

MF C18 H26 O2

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-[(1S)-2-bromo-1-ethoxyethoxy]-4,7-dimethoxy-2,5-dimethyl-6-[2-(phenylmethoxy)ethyl]-, (1S)- (9CI)

MF C26 H33 Br O5

Absolute stereochemistry. Rotation (+).

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Inden-1-ol, 2-methyl-3-phenyl-, acetate (9CI)
MF C18 H16 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Inden-1-ol, 6-methoxy-2-methyl-, acetate (9CI) MF C13 H14 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Indene, 1-methoxy-2-methyl-6-nitro- (9CI) MF C11 H11 N O3

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-methoxy-2,6-dimethyl- (9CI)

MF C12 H14 O

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 2,3-diethyl-1,5,7-trimethoxy- (9CI)

MF C16 H22 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 6-chloro-3-(4-chlorophenyl)-1-ethoxy-2-(2-ethoxyethyl)- (9CI)

MF C21 H22 C12 O2

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1H-Indene, 7-[(1,1-dimethylethoxy)methyl]-2,3-diethyl-1-methoxy- (9CI)
MF C19 H28 O2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Indene, 2,3-diethyl-1,5-dimethoxy- (9CI) MF C15 H20 O2

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Indene, 1-[(1R)-2-bromo-1-ethoxyethoxy]-4,7-dimethoxy-2,5-dimethyl-6-[2-(phenylmethoxy)ethyl]-, (1S)- (9CI)

MF C26 H33 Br O5

Absolute stereochemistry. Rotation (+).

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L6 68 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Inden-1-ol, 2-ethyl-3-phenyl-, acetate (9CI) MF C19 H18 O2

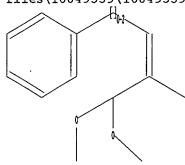
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

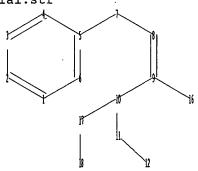
# ALL ANSWERS HAVE BEEN SCANNED

=> save temp prodcmpds/a
ENTER L#, L# RANGE, ALL, OR (END):16
ANSWER SET L6 HAS BEEN SAVED AS 'PRODCMPDS/A'

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10849559\10849559 starting material.str





chain nodes : 7 8 9 10 11 16 17

ring nodes :
1 2 3 4 5 6
ring/chain nodes :

12 18

chain bonds :

5-7 7-8 8-9 9-10 9-16 10-11 10-17 11-12 17-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

10-11 10-17 11-12 17-18

exact bonds :

5-7 7-8 8-9 9-10 9-16

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Hydrogen count :

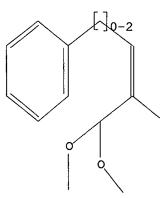
7:>= minimum 2 10:>= minimum 1

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 16:CLASS 17:CLASS 18:CLASS

#### L7 STRUCTURE UPLOADED

=> d 17 L7 HAS NO ANSWERS L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 17 sss sam
SAMPLE SEARCH INITIATED 06:59:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 187 TO ITERATE

100.0% PROCESSED 187 ITERATIONS 1 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2920 TO 4560 PROJECTED ANSWERS: 1 TO 80

L9 1 SEA SSS SAM L7

=> d scan

=>

L9 1 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2H-Pyran, 2-[2-[2-(diethoxymethyl)-4-phenyl-1,3-butadienyl]phenoxy]tetrahydro-, (Z,E)- (9CI)
MF C26 H32 O4

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> search 17 sss full FULL SEARCH INITIATED 06:59:58 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 3935 TO ITERATE

100.0% PROCESSED 3935 ITERATIONS 48 ANSWERS SEARCH TIME: 00.00.01

L10 48 SEA SSS FUL L7

=> d scan

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 2-Propenal, 2-(diethoxymethyl)-3-phenyl-, (2E)- (9CI) MF C14 H18 O3

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):48

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-4-ethoxy- (9CI)
MF C20 H32 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenenitrile, 3-(1,3-benzodioxol-5-yl)-2-(dimethoxymethyl)- (9CI)
MF C13 H13 N O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Propenenitrile, 3-(3-bromo-4,5-dimethoxyphenyl)-2-(dimethoxymethyl)(9CI)

MF C14 H16 Br N O4

$$\begin{array}{c|cccc} {\tt Ph-CH_2-CH_2-O} & {\tt CH-Ph} \\ & & | & || \\ {\tt Ph-CH_2-CH_2-O-CH-C-(CH_2)} \, {\tt 5-Me} \end{array}$$

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-4-(1-methylethyl)- (9CI)
MF C21 H34 O2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-chloro-4-[2-(diethoxymethyl)-3,3-diethoxy-1-propenyl]- (9CI)
MF C18 H27 C1 O4

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenoic acid, 2-(diethoxymethyl)-3-phenyl-, ethyl ester, (2Z)- (9CI)
MF C16 H22 O4

Double bond geometry as shown.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 2-Propenenitrile, 2-(dimethoxymethyl)-3-phenyl- (9CI) MF C12 H13 N O2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-2-ethyl- (9CI)
MF C20 H32 O2

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, (3,3-dibutoxy-2-methyl-1-propenyl)- (9CI) MF C18 H28 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Cinnamaldehyde,  $\beta\text{-chloro-}\alpha\text{-methyl-m-nitro-}$ , dimethyl acetal (7CI, 8CI) MF C12 H14 Cl N O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, [2-(bromomethyl)-3,3-diethoxy-1-propenyl]-, (Z)- (9CI)
MF C14 H19 Br O2

Double bond geometry as shown.

$$\begin{array}{c|c} \text{OEt} \\ \hline \\ \text{Eto} \\ \hline \\ \text{CH}_2\text{Br} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-2-methoxy- (9CI)
MF C19 H30 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Propenenitrile, 2-(dibutoxymethyl)-3-(4,5-dimethoxy-2-methylphenyl)(9CI)

MF C21 H31 N O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Malonaldehydonitrile, (p-chlorobenzylidene)-, dimethyl acetal (8CI)
MF C12 H12 Cl N O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 2-Propene-1,1-diol, 2-methyl-3-phenyl-, diacetate, (2E)- (9CI) MF C14 H16 O4

Double bond geometry as shown.

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, [(1E)-3,3-dimethoxy-2-methyl-1-propenyl]- (9CI) MF C12 H16 O2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-2-methyl- (9CI) MF C19 H30 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, [2-[bis[(1-ethenyl-1,5-dimethyl-4-hexenyl)oxy]methyl]-1-heptenyl](9CI)
MF C34 H52 O2

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, (3,3-dimethoxy-2-methyl-1-propenyl)- (9CI) MF C12 H16 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-4-ethyl- (9CI)
MF C20 H32 O2

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenamide, 3-[4-(3,3-diethoxy-2-methyl-1-propenyl)phenyl]-N-(1,1-dimethylethyl)-, (E,E)- (9CI)
MF C21 H31 N O3

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenenitrile, 2-(dimethoxymethyl)-3-(3,4-dimethoxyphenyl)- (9CI)
MF C14 H17 N O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 4-Pentenenitrile, 4-(diethoxymethyl)-2-[2-(diethoxymethyl)-3-phenyl-2-propenyl]-5-phenyl-, (E,E)- (9CI)

MF C30 H39 N O4

Double bond geometry as shown.

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-4-methoxy- (9CI)
MF C19 H30 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, [2-(diethoxymethyl)-3,3-diethoxy-1-propenyl]- (9CI)
MF C18 H28 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenenitrile, 3-[4-(diethylamino)-2-methoxyphenyl]-2-(dimethoxymethyl)(9CI)
MF C17 H24 N2 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1,4-Pentadien-3-ol, 2,4-bis(diethoxymethyl)-1,5-diphenyl-, (1E,4E)- (9CI)
MF C27 H36 O5

Double bond geometry as shown.

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, (3,3-diethoxy-2-methyl-1-propenyl)- (9CI) MF C14 H20 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-4-methyl- (9CI)
MF C19 H30 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, [2-(diethoxymethyl)-1-octenyl]- (9CI) MF C19 H30 O2

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 2-Propene-1,1-diol, 2-methyl-3-phenyl-, diacetate (9CI) MF C14 H16 O4

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Acetamide, N-[2-[2-(diethoxymethyl)-4-(trimethylsilyl)-1,3-butadienyl]phenyl]-, (E,Z)- (9CI)
MF C20 H31 N O3 Si

Double bond geometry as shown.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-2-ethoxy- (9CI)
MF C20 H32 O3

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenenitrile, 2-(dimethoxymethyl)-3-(4,5-dimethoxy-2-methylphenyl)(9CI)
MF C15 H19 N O4

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenenitrile, 2-(dimethoxymethyl)-3-(3,4,5-trimethoxyphenyl)- (9CI)
MF C15 H19 N O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 2H-Pyran, 2-[2-[2-(diethoxymethyl)-4-phenyl-1,3-butadienyl]phenoxy]tetrahydro-, (Z,E)- (9CI) MF C26 H32 O4

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-2-(1-methylethyl)- (9CI)
MF C21 H34 O2

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzene, 1-[2-(diethoxymethyl)-3,3-diethoxy-1-propenyl]-4-methoxy- (9CI)

MF C19 H30 O5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, [2-(diethoxymethyl)-1-heptenyl]- (9CI) MF C18 H28 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, [2-[bis(1-methylethoxy)methyl]-1-heptenyl]- (9CI)
MF C20 H32 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, (3,3-diethoxy-2-methyl-1-propenyl)-, (E)- (9CI) MF C14 H20 O2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzene, 1-(3,3-dibutoxy-2-methyl-1-propenyl)-3,5-dimethyl- (9CI)
MF C20 H32 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, [2-(dimethoxymethyl)-1-octenyl]- (9CI) MF C17 H26 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 48 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Benzene, [2-(dimethoxymethyl)-1-heptenyl]- (9CI) MF C16 H24 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> save temp 110 stmatfnds/a
ANSWER SET L10 HAS BEEN SAVED AS 'STMATFNDS/A'

#### => d his

(FILE 'HOME' ENTERED AT 06:32:16 ON 25 JUL 2006)

FILE 'REGISTRY' ENTERED AT 06:42:20 ON 25 JUL 2006 STRUCTURE UPLOADED . L1 0 SEARCH L1 SSS SAM L2L3 82 SEARCH L1 SSS FULL L40 DSCAN SAVE TEMP L3 RAWHETROS/A STRUCTURE UPLOADED T.5 68 SEARCH L5 SSS FULL SUB=L3 L6 SAVE TEMP PRODCMPDS/A L6 STRUCTURE UPLOADED L7 0 SEARCHL7 SSS SAM  $^{18}$ 1 SEARCH L7 SSS SAM L9 L10 48 SEARCH L7 SSS FULL SAVE TEMP L10 STMATFNDS/A

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 396.00 396.63

FULL ESTIMATED COST

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=> 16

L11 31 L6

=> 110

L12 57 L10

=> 16 and 110

31 L6 57 L10

L13 , 1 L6 AND L10

- L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Catalytic cyclocondensation process for producing indenol esters or ethers from an  $\alpha$ -substituted cinnamic aldehyde acetal or or an acylal
- AN 2005:1242659 CAPLUS
- DN 144:6579
- TI Catalytic cyclocondensation process for producing indenol esters or ethers from an  $\alpha$ -substituted cinnamic aldehyde acetal or or an acylal
- IN Womack, Gary Bernard; Snowden, Roger Lesile; Mosimann, Herve
- PA USA
- SO U.S. Pat. Appl. Publ., 6 pp.
- CODEN: USXXCO
- DT Patent
- LA English
- FAN.CNT 1

LTM.		TENT 1	NO.			KIND DATE			APPLICATION NO.						DATE			
PI	WO	US 2005261513 WO 2005113473 WO 2005113473				A1 20051124 A2 20051201 A3 20060413			US 2004-849559 WO 2005-IB1474						20040518 20050510			
		W:	CN, GE, LC, NG, SL,	CO, GH, LK, NI,	CR, GM, LR, NO, SY,	CU, HR, LS, NZ,	CZ, HU, LT, OM,	AU, DE, ID, LU, PG, TN,	DK, IL, LV, PH,	DM, IN, MA, PL,	DZ, IS, MD, PT,	EC, JP, MG, RO,	EE, KE, MK, RU,	EG, KG, MN, SC,	ES, KM, MW, SD,	FI, KP, MX, SE,	GB, KR, MZ, SG,	GD, KZ, NA, SK,
		RW:	BW, AZ, EE, RO,	GH, BY, ES, SE,	GM, KG, FI, SI,	KZ, FR,	MD, GB, TR,	MW, RU, GR, BF,	TJ, HU,	TM, IE, CF,	AT, IS, CG,	BE, IT, CI,	BG, LT, CM,	CH, LU,	CY, MC, GN,	CZ, NL, GQ,	DE, PL,	DK, PT, ML,

OS CASREACT 144:6579; MARPAT 144:6579

AB A process is described for making indenol esters or ethers (e.g., 1-methoxy-2-methyl-1H-indene; b.p.  $32-43^{\circ}/0.07$  mbar) from an  $\alpha$ -substituted cinnamic aldehyde derivative such as an acetal (e.g., 3,3-dimethoxy-2-methyl-1-phenyl-1-propene) or an acytal in the presence of catalysts which are strong mineral acids, sulfonic acids, acidic zeolites, or Lewis acids (e.g., ferric chloride).

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	4.12	400.75
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
•	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.75	-0.75

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:03:33 ON 25 JUL 2006

Connecting via Winsock to STN

### LOGINID: SSSPTA1623PAZ

### PASSWORD:

\* \* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* SESSION RESUMED IN FILE 'CAPLUS' AT 07:30:35 ON 25 JUL 2006 FILE 'CAPLUS' ENTERED AT 07:30:35 ON 25 JUL 2006 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS FULL ESTIMATED COST	SINCE FILE ENTRY 4.12	TOTAL SESSION 400.75
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.75	-0.75
=> logoff hold COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.58	401.21
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.75	-0.75

SESSION WILL BE HELD FOR 60 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 07:31:01 ON 25 JUL 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

#### PASSWORD:

\* \* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* \* SESSION RESUMED IN FILE 'CAPLUS' AT 07:35:48 ON 25 JUL 2006 FILE 'CAPLUS' ENTERED AT 07:35:48 ON 25 JUL 2006 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS FULL ESTIMATED COST	SINCE FILE ENTRY 4.58	TOTAL SESSION 401.21
ENTRY 4.58  DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE ENTRY -0.75  FOR THE PRICE  SINCE FILE ENTRY -0.75  FULL ESTIMATED COST  DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE ENTRY 4.58  DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE ENTRY		TOTAL SESSION -0.75
=> file reg COST IN U.S. DOLLARS FULL ESTIMATED COST	ENTRY	TOTAL SESSION 401.21
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) CA SUBSCRIBER PRICE	ENTRY	TOTAL SESSION -0.75

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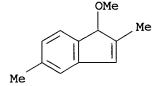
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> e 1H-Indene, 1-methoxy-2,5-dimethyl-/cn

```
1H-INDENE, 1-METHOXY-2, 3-DIPHENYL-/CN
E1
             1
                   1H-INDENE, 1-METHOXY-2, 4-DIMETHYL-/CN
E2
             1 --> 1H-INDENE, 1-METHOXY-2,5-DIMETHYL-/CN
E3
                   1H-INDENE, 1-METHOXY-2,6-DIMETHYL-/CN
E4
             1
                   1H-INDENE, 1-METHOXY-2,7-DIMETHYL-/CN
E5
             1
                   1H-INDENE, 1-METHOXY-2-METHYL-/CN
             1
E6
                   1H-INDENE, 1-METHOXY-2-METHYL-6-NITRO-/CN
             1
E7
                   1H-INDENE, 1-METHOXY-2-NITRO-3-PHENYL-/CN
E8
             1
                   1H-INDENE, 1-METHOXY-3-METHYL-/CN
E9
             1
                   1H-INDENE, 1-METHOXY-7-(1-PROPENYLOXY)-/CN
E10
             1
                   1H-INDENE, 1-METHYL-/CN
E11
             1
E12
                   1H-INDENE, 1-METHYL-, (R)-/CN
=> e3
L14
             1 "1H-INDENE, 1-METHOXY-2,5-DIMETHYL-"/CN
=> d 114
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
L14
     894779-05-6 REGISTRY
RN
     Entered STN: 20 Jul 2006
ED
     1H-Indene, 1-methoxy-2,5-dimethyl- (9CI) (CA INDEX NAME)
CN
FS
     3D CONCORD
MF
     C12 H14 O
SR
     CA
     STN Files:
                  CAPLUS
LC
```



1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION FULL ESTIMATED COST 7.10 408.31 SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) ENTRY SESSION 0.00 -0.75CA SUBSCRIBER PRICE

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=>

=> 114

L15

1 L14

=> d l15 ti fbib abs

L15 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

- TI Intramolecular electrophilic aromatic substitution of  $\alpha$ -alkylcinnamaldehydes affording 1-alkoxy-2-alkylindenes
- AN 2006:478943 CAPLUS
- TI Intramolecular electrophilic aromatic, substitution of  $\alpha$ -alkylcinnamaldehydes affording 1-alkoxy-2-alkylindenes
- AU Jobashi, Takashi; Kawai, Atsushi; Kawai, Satomi; Maeyama, Katsuya; Oike, Hideaki; Yoshida, Yasuhiko; Yonezawa, Noriyuki
- CS Department of Organic and Polymer Materials Chemistry, Tokyo University of Agriculture & Technology, Koganei, Tokyo, 184-8588, Japan
- SO Tetrahedron (2006), 62(24), 5717-5724 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier B.V.
- DT Journal
- LA English
- AB Treatment of  $\alpha$ -alkylcinnamaldehydes with orthoesters, alcs., or thiols in the presence of BF3·OEt2 induces an intramol. electrophilic aromatic substitution reaction to afford 1-alkoxy-2-alkylindenes. The reaction mechanisms of the indene formation have been elucidated on the basis of the reaction behaviors of  $\beta$ -deuterated  $\alpha$ -methylcinnamaldehyde and the NMR studies of the reaction mixture The transformation process involves successive reactions, i.e., alkoxylation of the carbonyl carbon of  $\alpha$ -alkylcinnamaldehydes to form acetals, elimination of alkoxide from the acetals to give

alkoxycarbenium ion and  $\gamma$ -alkoxyallyl cation, and intramol. electrophilic arylation to afford the indene ring structure. THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold COST IN U.S. DOLLARS

TOTAL
SESSION
6.42 SINCE FILE TOTAL ENTRY

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

-0.75 -1.50

SESSION WILL BE HELD FOR 60 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 07:41:03 ON 25 JUL 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

### PASSWORD:

\* \* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* SESSION RESUMED IN FILE 'CAPLUS' AT 07:50:06 ON 25 JUL 2006 FILE 'CAPLUS' ENTERED AT 07:50:06 ON 25 JUL 2006 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

TOTAL COST IN U.S. DOLLARS SINCE FILE ENTRY SESSION FULL ESTIMATED COST 6.42 414.73 TOTAL DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS) SINCE FILE ENTRY SESSION -0.75CA SUBSCRIBER PRICE -1.50

=> d his

(FILE 'HOME' ENTERED AT 06:32:16 ON 25 JUL 2006)

FILE 'REGISTRY' ENTERED AT 06:42:20 ON 25 JUL 2006

STRUCTURE UPLOADED L10 SEARCH L1 SSS SAM L2 L3 82 SEARCH L1 SSS FULL

L40 DSCAN

SAVE TEMP L3 RAWHETROS/A

L5 STRUCTURE UPLOADED

L6 68 SEARCH L5 SSS FULL SUB=L3 SAVE TEMP PRODCMPDS/A L6

STRUCTURE UPLOADED L7

0 SEARCHL7 SSS SAM L8 1 SEARCH L7 SSS SAM

L9 48 SEARCH L7 SSS FULL L10

SAVE TEMP L10 STMATFNDS/A

FILE 'CAPLUS' ENTERED AT 07:01:48 ON 25 JUL 2006

T.11 31 L6 L12 57 L10 L13 1 L6 AND L10

FILE 'REGISTRY' ENTERED AT 07:36:02 ON 25 JUL 2006 E 1H-INDENE, 1-METHOXY-2,5-DIMETHYL-/CN

L14 1 E3

FILE 'CAPLUS' ENTERED AT 07:36:30 ON 25 JUL 2006 L15 1 L14

=> file reg

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
6.88
415.19

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

-0.75
-1.50

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STRUCTURE FILE UPDATES: 21 JUL 2006 HIGHEST RN 894992-91-7 DICTIONARY FILE UPDATES: 21 JUL 2006 HIGHEST RN 894992-91-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

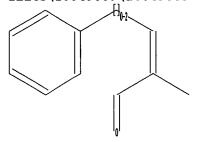
TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

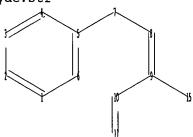
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10849559\10849559 starting aldehyde.str





chain nodes :
7 8 9 10 11 15
ring nodes :
1 2 3 4 5 6
chain bonds :
5-7 7-8 8-9 9-10 9-15 10-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds:

10-11

exact bonds :

5-7 7-8 8-9 9-10 9-15

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Hydrogen count :

7:>= minimum 2 10:>= minimum 1

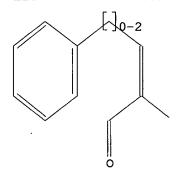
Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:CLASS 15:CLASS

L16 STRUCTURE UPLOADED

=> d 116 L16 HAS NO ANSWERS L16 STR



Structure attributes must be viewed using STN Express query preparation.

9 ANSWERS

=> search 116 sss sam
SAMPLE SEARCH INITIATED 07:51:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 11549 TO ITERATE

17.3% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 224541 TO 237419
PROJECTED ANSWERS: 607 TO 1471

L17 9 SEA SSS SAM L16

=> d scan

L17 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 2-Propenal, 3-(2,4-dimethoxyphenyl)-2-methyl- (9CI) MF C12 H14 O3

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L17 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenenitrile, 3-amino-2-formyl-3-(2-naphthalenyl)-, (Z)- (9CI)
MF C14 H10 N2 O

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L17 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenenitrile, 3-(2,4-dichlorophenyl)-2-formyl- (9CI)
MF C10 H5 C12 N O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Double bond geometry as shown.

L17 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzenebutanal,  $\beta$ -(dimethoxymethylene)- $\alpha$ -(diphenylmethylene)- $\gamma$ -phenyl- (9CI)

MF C32 H28 O3

$$\begin{array}{c|c} {\tt Ph_2C} & {\tt CHPh_2} \\ \parallel & \parallel \\ {\tt OHC-C-C} & = {\tt C-OMe} \\ \parallel & \parallel \\ & {\tt OMe} \end{array}$$

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L17 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzoic acid, 2-hydroxy-4-methoxy-5-methyl-3-(3-methyl-4-oxo-2-butenyl)-,
 methyl ester, (E)- (9CI)
MF C15 H18 O5

Double bond geometry as shown.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L17 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Propenal, 3-[4-(4-chlorophenoxy)phenyl]-2-methyl- (9CI)
MF C16 H13 Cl O2

L17 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 2-Propenenitrile, 2-formyl-3-(4-methylphenyl)- (9CI) MF C11 H9 N O

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L17 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Naphthalenesulfonic acid, 4-amino-3-[[4-(2-methyl-3-oxo-1-propenyl)phenyl]azo]-, monosodium salt (9CI)
MF C20 H17 N3 O4 S . Na

Na

ALL ANSWERS HAVE BEEN SCANNED

=> search 116 sss full FULL SEARCH INITIATED 07:51:51 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 230880 TO ITERATE

100.0% PROCESSED 230880 ITERATIONS SEARCH TIME: 00.00.03

940 ANSWERS

L18 940 SEA SSS FUL L16

=> save temp 118 staldfnds/a

### ANSWER SET L18 HAS BEEN SAVED AS 'STALDFNDS/A'

=> file caplus SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION FULL ESTIMATED COST 167.82 583.01 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -1.50

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FILE COVERS 1907 - 25 Jul 2006 VOL 145 ISS 5 FILE LAST UPDATED: 24 Jul 2006 (20060724/ED)

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http://www.cas.org/infopolicy.html

=> d his

(FILE 'HOME' ENTERED AT 06:32:16 ON 25 JUL 2006)

```
FILE 'REGISTRY' ENTERED AT 06:42:20 ON 25 JUL 2006
                STRUCTURE UPLOADED
L1
              0 SEARCH L1 SSS SAM
L2
L3
             82 SEARCH L1 SSS FULL
T.4
              0 DSCAN
                SAVE TEMP L3 RAWHETROS/A
                STRUCTURE UPLOADED
L5
             68 SEARCH L5 SSS FULL SUB=L3
L6
                SAVE TEMP PRODCMPDS/A L6
                STRUCTURE UPLOADED
L7
L8
              0 SEARCHL7 SSS SAM
L9
             1 SEARCH L7 SSS SAM
L10
             48 SEARCH L7 SSS FULL
                SAVE TEMP L10 STMATFNDS/A
     FILE 'CAPLUS' ENTERED AT 07:01:48 ON 25 JUL 2006
             31 L6
L11
             57 L10
L12
              1 L6 AND L10
T<sub>1</sub>13
```

FILE 'REGISTRY' ENTERED AT 07:36:02 ON 25 JUL 2006 E 1H-INDENE, 1-METHOXY-2,5-DIMETHYL-/CN

L14 1 E3

```
FILE 'CAPLUS' ENTERED AT 07:36:30 ON 25 JUL 2006
L15
              1 L14
     FILE 'REGISTRY' ENTERED AT 07:50:32 ON 25 JUL 2006
                STRUCTURE UPLOADED
L16
L17
              9 SEARCH L16 SSS SAM
L18
            940 SEARCH L16 SSS FULL
                SAVE TEMP L18 STALDFNDS/A
     FILE 'CAPLUS' ENTERED AT 07:52:32 ON 25 JUL 2006
=> 118
L19
          1934 L18
=> 13 and 119
            38 L3
             3 L3 AND L19
L20
=> d 120 1-3 ti fbib abs
L20 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
     Intramolecular electrophilic aromatic substitution of \alpha-
     alkylcinnamaldehydes affording 1-alkoxy-2-alkylindenes
     2006:478943 CAPLUS
ΑN
     Intramolecular electrophilic aromatic substitution of \alpha-
ΤI
     alkylcinnamaldehydes affording 1-alkoxy-2-alkylindenes
ΑU
     Jobashi, Takashi; Kawai, Atsushi; Kawai, Satomi; Maeyama, Katsuya; Oike,
     Hideaki; Yoshida, Yasuhiko; Yonezawa, Noriyuki
CS
     Department of Organic and Polymer Materials Chemistry, Tokyo University of
     Agriculture & Technology, Koganei, Tokyo, 184-8588, Japan
     Tetrahedron (2006), 62(24), 5717-5724
SO
     CODEN: TETRAB; ISSN: 0040-4020
PB
     Elsevier B.V.
DT
     Journal
LΑ
     English
AB
     Treatment of \alpha-alkylcinnamaldehydes with orthoesters, alcs., or
     thiols in the presence of BF3.OEt2 induces an intramol.
     electrophilic aromatic substitution reaction to afford 1-alkoxy-2-
     alkylindenes. The reaction mechanisms of the indene formation have been
     elucidated on the basis of the reaction behaviors of \beta\text{-deuterated}
     \alpha-methylcinnamaldehyde and the NMR studies of the reaction mixture
     The transformation process involves successive reactions, i.e.,
     alkoxylation of the carbonyl carbon of \alpha-alkylcinnamaldehydes to
     form acetals, elimination of alkoxide from the acetals to give
     alkoxycarbenium ion and \gamma-alkoxyallyl cation, and intramol.
     electrophilic arylation to afford the indene ring structure.
              THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 43
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
L20
ΤI
     Catalytic cyclocondensation process for producing indenol esters or ethers
     from an \alpha-substituted cinnamic aldehyde acetal or or an acylal
ΑN
     2005:1242659 CAPLUS
DN
     144:6579
     Catalytic cyclocondensation process for producing indenol esters or ethers
ΤI
     from an \alpha-substituted cinnamic aldehyde acetal or or an acylal
     Womack, Gary Bernard; Snowden, Roger Lesile; Mosimann, Herve
IN
PA
SO
     U.S. Pat. Appl. Publ., 6 pp.
     CODEN: USXXCO
DT
     Patent
LΆ
     English
FAN.CNT 1
```

PATENT	PATENT NO.						APPLICATION NO.						DATE		
WO 2005	US 2005261513 WO 2005113473 WO 2005113473		A1 20051124 A2 20051201 A3 20060413								20040518 20050510				
₩:		CR, GM, LR, NO, SY, ZW GM, KG, FI,	AM, CU, HR, LS, NZ, TJ, KE, KZ, FR, SK,	AT, CZ, HU, LT, OM, TM, LS, MD, GB, TR,	AU, DE, ID, LU, PG, TN, MW, RU, GR,	AZ, DK, IL, LV, PH, TR, MZ, TJ,	DM, IN, MA, PL, TT, NA, TM, IE, CF,	DZ, IS, MD, PT, TZ, SD, AT, IS,	EC, JP, MG, RO, UA, SL, BE, IT, CI,	EE, KE, MK, RÚ, UG, SZ, BG, LT, CM,	EG, KG, MN, SC, US, TZ, CH, LU, GA,	ES, KM, MW, SD, UZ, UG, CY, MC, GN,	FI, KP, MX, SE, VC, ZM, CZ, NL,	GB, KR, MZ, SG, VN, ZW, DE, PL, GW,	GD, KZ, NA, SK, YU, AM, DK, PT, ML,

OS CASREACT 144:6579; MARPAT 144:6579

AB A process is described for making indenol esters or ethers (e.g., 1-methoxy-2-methyl-1H-indene; b.p.  $32-43^{\circ}/0.07$  mbar) from an  $\alpha$ -substituted cinnamic aldehyde derivative such as an acetal (e.g., 3,3-dimethoxy-2-methyl-1-phenyl-1-propene) or an acytal in the presence of catalysts which are strong mineral acids, sulfonic acids, acidic zeolites, or Lewis acids (e.g., ferric chloride).

L20 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

TI Preparation of indan derivatives as antiasthmatic agents

AN 1990:98228 CAPLUS

DN 112:98228

TI Preparation of indan derivatives as antiasthmatic agents

IN Ohira, Kazuo; Imai, Eiji; Nakaoku, Shozo; Nagai, Hiroichi

PA Taiyo Yakuhin Kogyo K. K., Japan

SO Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		- <b></b>			
PI	JP 63005063	A2	19880111	JP 1986-148289 JP 1986-148289	19860626 19860626

OS CASREACT 112:98228; MARPAT 112:98228 GI

Ι

$$0 \longrightarrow Bu$$

AB Indan derivs. [I; R1 = alkyl; R2,R3 = alkyl, R2R3 = alkylene; R4,R5 = (substituted) alkyl or aryl, R4R5N = piperidino, piperazinyl, homopiperazinyl, R4 = R5 ≠ Me], useful as antiasthmatic agents, are prepared Reaction of bromoindene derivative II (R6 = Br) with Me2NCH2CH2NHMe and Na2CO3 in Me2SO gave 68% amination product II (R6 = Me2NCH2CH2NMe), which as the HCl salt (3.8 g) was hydrogenated over PtO2 in EtOH to give 1.4 g cis- and 62 mg trans-I (R1 = Bu, R2R3 = CH2, R4 = Me, R5 = Me2NCH2CH2), which showed bronchi contraction inhibition at 5 + 10-5

ΙI

=> d cost	•	
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
CONNECT CHARGES	2.40	21.73
NETWORK CHARGES	0.36	3.48
SEARCH CHARGES	0.00	553.18
DISPLAY CHARGES	8.22	15.60
FULL ESTIMATED COST	10.98	593.99
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.25	-3.75

IN FILE 'CAPLUS' AT 07:56:16 ON 25 JUL 2006

=> save temp all indenylsrch/a
'INDENYLSRCH/A' IS NOT ALLOWED WITH ALL
The saved name of an L# list must end with '/L'.

=> save temp all indenylsrch/l
L# LIST L1-L20 HAS BEEN SAVED AS 'INDENYLSRCH/L'

=> logoff hold SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION 12.36 595.37 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION -3.75CA SUBSCRIBER PRICE -2.25

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:57:47 ON 25 JUL 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* \* \* SESSION RESUMED IN FILE 'CAPLUS' AT 08:09:14 ON 25 JUL 2006 FILE 'CAPLUS' ENTERED AT 08:09:14 ON 25 JUL 2006 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	12.36	595.37
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.25	-3.75

# (FILE 'HOME' ENTERED AT 06:32:16 ON 25 JUL 2006)

L1 L2 L3 L4 L5 L6 L7 L8 L9 L10	FILE	'REGISTRY' ENTERED AT 06:42:20 ON 25 JUL 20 STRUCTURE UPLOADED  0 SEARCH L1 SSS SAM 82 SEARCH L1 SSS FULL 0 DSCAN SAVE TEMP L3 RAWHETROS/A STRUCTURE UPLOADED 68 SEARCH L5 SSS FULL SUB=L3 SAVE TEMP PRODCMPDS/A L6 STRUCTURE UPLOADED 0 SEARCHL7 SSS SAM 1 SEARCH L7 SSS SAM 48 SEARCH L7 SSS FULL	06
пто		SAVE TEMP L10 STMATFNDS/A	
L11 L12 L13		'CAPLUS' ENTERED AT 07:01:48 ON 25 JUL 2006 31 L6 57 L10 1 L6 AND L10	
L14	FILE	'REGISTRY' ENTERED AT 07:36:02 ON 25 JUL 20 E 1H-INDENE, 1-METHOXY-2,5-DIMETHYL-/ 1 E3	
L15	FILE	'CAPLUS' ENTERED AT 07:36:30 ON 25 JUL 2006 1 L14	i
		'REGISTRY' ENTERED AT 07:50:32 ON 25 JUL 20 STRUCTURE UPLOADED 9 SEARCH L16 SSS SAM 940 SEARCH L16 SSS FULL SAVE TEMP L18 STALDFNDS/A	06
		'CAPLUS' ENTERED AT 07:52:32 ON 25 JUL 2006 1934 L18 3 L3 AND L19 SAVE TEMP ALL INDENYLSRCH/L	;·
	-	hold .s. DOLLARS SINC	E FILE
FULL	ESTIN	MATED COST	ENTRY 12.82

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 08:09:36 ON 25 JUL 2006

TOTAL SESSION 595.83

TOTAL

-3.75

SESSION

SINCE FILE ENTRY

-2.25

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

LOGINID: SSSPTA1623PAZ

CA SUBSCRIBER PRICE

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* \* SESSION RESUMED IN FILE 'CAPLUS' AT 08:16:14 ON 25 JUL 2006 FILE 'CAPLUS' ENTERED AT 08:16:14 ON 25 JUL 2006 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS FULL ESTIMATED COST	SINCE FILE ENTRY 12.82	TOTAL SESSION 595.83
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) . CA SUBSCRIBER PRICE	SINCE FILE ENTRY -2.25	TOTAL SESSION -3.75
=> file reg COST IN U.S. DOLLARS FULL ESTIMATED COST	SINCE FILE ENTRY 12.82	TOTAL SESSION 595.83
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  CA SUBSCRIBER PRICE	SINCE FILE ENTRY -2.25	TOTAL SESSION -3.75

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STRUCTURE FILE UPDATES: 23 JUL 2006 HIGHEST RN 895579-80-3 DICTIONARY FILE UPDATES: 23 JUL 2006 HIGHEST RN 895579-80-3

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>		2,6-dimethyl-, acetate/cn
E1	1	1H-INDEN-1-OL, 2,6,7,7A-TETRAHYDRO-7A-METHYL-5-(1-PYRROLIDIN
		YL)-, ACETATE (ESTER)/CN
E2	1	1H-INDEN-1-OL, 2,6,7-TRIFLUORO-2,3-DIHYDRO-, CIS-/CN
<b>E</b> 3	1>	1H-INDEN-1-OL, 2,6-DIMETHYL-, ACETATE/CN
E4	1	1H-INDEN-1-OL, 2-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-2,3
		-DIHYDRO-, CIS-/CN
E5	<u>1</u>	1H-INDEN-1-OL, 2-(((2,3-DIMETHOXYPHENYL)METHYL)AMINO)-2,3-DI
		HYDRO-, (1S-TRANS)-/CN
E6	1	1H-INDEN-1-OL, 2-(((2,3-DIMETHOXYPHENYL)METHYLENE)AMINO)-2,3
		-DIHYDRO-, (1S-TRANS)-/CN
E7	1	1H-INDEN-1-OL, 2-(((2,3-DIMETHOXYPHENYL)METHYLENE)AMINO)-2,3
		-DIHYDRO-5-METHOXY-, (1S-TRANS)-/CN
E8	1	1H-INDEN-1-OL, 2-(((3,4-DIMETHOXYPHENYL)METHYL)AMINO)-2,3-DI
		HYDRO-, (1S-TRANS)-/CN
E9	1	1H-INDEN-1-OL, 2-(((3,4-DIMETHOXYPHENYL)METHYL)AMINO)-2,3-DI

HYDRO-, HYDROCHLORIDE, (1S-TRANS)-/CN E10 1 1H-INDEN-1-OL, 2-(((3,4-DIMETHOXYPHENYL)METHYL)AMINO)-2,3-DI HYDRO-4,5-DIMETHOXY-, (1S-TRANS)-/CN 1H-INDEN-1-OL, 2-(((3,4-DIMETHOXYPHENYL)METHYL)AMINO)-2,3-DI 1 E11 HYDRO-4,5-DIMETHOXY-, HYDROCHLORIDE, (1S-TRANS)-/CN 1H-INDEN-1-OL, 2-(((3,4-DIMETHOXYPHENYL)METHYL)AMINO)-2,3-DI E12 1 HYDRO-5-METHOXY-, (1S-TRANS)-/CN => e31 "1H-INDEN-1-OL, 2,6-DIMETHYL-, ACETATE"/CN L21 => d 121

L21 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 870002-58-7 REGISTRY

ED Entered STN: 15 Dec 2005

CN 1H-Inden-1-ol, 2,6-dimethyl-, acetate (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H14 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION FULL ESTIMATED COST 7.10 602.93 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL SESSION ENTRY -3.75CA SUBSCRIBER PRICE 0.00

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FILE COVERS 1907 - 25 Jul 2006 VOL 145 ISS 5

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=> 121

1 L21 L22

=> d 122ti fbib abs

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#### => d 122 ti fbib abs

- L22 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Catalytic cyclocondensation process for producing indenol esters or ethers from an  $\alpha$ -substituted cinnamic aldehyde acetal or or an acylal
- AN 2005:1242659 CAPLUS
- DN 144:6579
- TI Catalytic cyclocondensation process for producing indenol esters or ethers from an  $\alpha$ -substituted cinnamic aldehyde acetal or or an acylal
- IN Womack, Gary Bernard; Snowden, Roger Lesile; Mosimann, Herve
- PA USA
- SO U.S. Pat. Appl. Publ., 6 pp. CODEN: USXXCO
- DT Patent
- LA English

### FAN.CNT 1

	PATENT NO.					KIND DATE			APPLICATION NO.						DATE			
ΡI	US	2005	2615	13		A1	A1 20051124		US 2004-849559						20040518			
	WO	2005	005113473			<b>A</b> 2	2 20051201			WO 2005-IB1474						20050510		
	WO	2005	2005113473			A3 20060413												
	W: AE, AG,		AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	ÇН,		
			CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	ΚP,	KR,	ΚZ,
			LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	ΜX,	ΜZ,	NA,
			NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,
			SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ΥU,
			ZA,	ZM,	zw													
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
			ΑZ,	BY,	KG,	KZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
			ΕĖ,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
			RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
			MR,	NE,	SN,	TD,	TG											
	MR, NE, SN, TD, TG							US 2004-849559					1	A 20040518				

OS CASREACT 144:6579; MARPAT 144:6579

AB A process is described for making indenol esters or ethers (e.g., 1-methoxy-2-methyl-1H-indene; b.p.  $32-43^{\circ}/0.07$  mbar) from an  $\alpha$ -substituted cinnamic aldehyde derivative such as an acetal (e.g., 3,3-dimethoxy-2-methyl-1-phenyl-1-propene) or an acytal in the presence of catalysts which are strong mineral acids, sulfonic acids, acidic zeolites, or Lewis acids (e.g., ferric chloride).

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
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FULL ESTIMATED COST	3.20	606.13
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
PIBODONI INDONIS (ION GOIMILIAMO NOCONIS)	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.75	-4.50

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•	ENTRY	SESSION
FULL ESTIMATED COST	3.20	606.13
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.75	-4.50

=> d his

(FILE 'HOME' ENTERED AT 06:32:16 ON 25 JUL 2006)

	FILE	'REGISTRY' ENTERED AT 06:42:20 ON 25 JUL 2006
L1		STRUCTURE UPLOADED
L2		0 SEARCH L1 SSS SAM
L3		82 SEARCH L1 SSS FULL
L4		0 DSCAN
		SAVE TEMP L3 RAWHETROS/A
L5		STRUCTURE UPLOADED
L6		68 SEARCH L5 SSS FULL SUB=L3
	•	SAVE TEMP PRODCMPDS/A L6
L7		STRUCTURE UPLOADED
L8		0 SEARCHL7 SSS SAM
L9		1 SEARCH L7 SSS SAM
L10		48 SEARCH L7 SSS FULL
		SAVE TEMP L10 STMATFNDS/A
	FILE	'CAPLUS' ENTERED AT 07:01:48 ON 25 JUL 2006
L11		31 L6
T 1 2		67 T10

57 L10 L12

L13 1 L6 AND L10

FILE 'REGISTRY' ENTERED AT 07:36:02 ON 25 JUL 2006 E 1H-INDENE, 1-METHOXY-2,5-DIMETHYL-/CN

L14 1 E3

FILE 'CAPLUS' ENTERED AT 07:36:30 ON 25 JUL 2006 L15 1 L14

FILE 'REGISTRY' ENTERED AT 07:50:32 ON 25 JUL 2006

L16 STRUCTURE UPLOADED L17 9 SEARCH L16 SSS SAM

L18 940 SEARCH L16 SSS FULL

SAVE TEMP L18 STALDFNDS/A

FILE 'CAPLUS' ENTERED AT 07:52:32 ON 25 JUL 2006

L19 1934 L18

L20 3 L3 AND L19

SAVE TEMP ALL INDENYLSRCH/L

FILE 'REGISTRY' ENTERED AT 08:16:25 ON 25 JUL 2006

E 1H-INDEN-1-OL, 2,6-DIMETHYL-, ACETATE/CN

L21 1 E3

FILE 'CAPLUS' ENTERED AT 08:17:17 ON 25 JUL 2006

L22 1 L21

=> logoff hold

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SESSION ENTRY 3.20 FULL ESTIMATED COST 606.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

ENTRY SESSION -0.75 -4.50 CA SUBSCRIBER PRICE

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